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Electronic Structure of Magnetite

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Magnetite Fe_3O_4 is a ferrimagnet (T_C=860 K) with a spinel structure. Iron occupies two sublattices - octahedral (B) and tetrahedral (A). The formal ionic distribution is $(Fe^{3+})_A(Fe^{3+}Fe^{2+})_BO_4^{2-}$ i.e. there is a mixed valence of Fe on the octahedral sublattice. The electronic structure of magnetite in its cubic phase (above the Verwey transition) is still matter of discussion, as it is not clear whether the charge carriers are small polarons or itinerant electrons.

Using the FP LAPW method, as implemented in the WIEN97 package, with recently added LDA+U option, the electron structure of magnetite in its cubic phase is calculated. The LSDA results are close to those recently obtained by Yanase and Hamada, total spin magnetic moment per unit cell 4.00 μ_B agrees well with the experimental total magnetic moment 4.05-4.12 μ_B. The magnetic moment of tetrahedral iron is smaller, however, than the neutron diffraction result. Using the LDA+U scheme, the sublattice moments are increased, while their sum remains unchanged, so that the agreement with the experiment is improved. Both LSDA and LDA+U show that magnetite is an ideal halfmetal - the Fermi energy intersects the minority spin $3d$ band of octahedral irons, while for the majority spin bands a gap exists, magnitude of which increases with increasing parameter U. Using both LSDA and LDA+U we also calculate the magneto-optical effects and hyperfine fields and compare the results with the experiment.